

# Yang-Lee edge singularities from extended activity expansions of the dimer density for bipartite lattices of dimensionality $2 \leq d \leq 7$

P. Butera\*

*Dipartimento di Fisica Universita' di Milano-Bicocca  
and  
Istituto Nazionale di Fisica Nucleare  
Sezione di Milano-Bicocca  
3 Piazza della Scienza,  
20126 Milano, Italy*

M. Pernici†

*Istituto Nazionale di Fisica Nucleare  
Sezione di Milano  
16 Via Celoria, 20133 Milano, Italy  
(Dated: June 6, 2012)*

## Abstract

We have extended, in most cases through 24th order, the series expansions of the dimer density in powers of the activity in the case of bipartite ((hyper)-simple-cubic and (hyper)-body-centered-cubic) lattices of dimensionalities  $2 \leq d \leq 7$ . A numerical analysis of these data yields estimates of the exponents characterizing the Yang-Lee edge-singularities for lattice ferromagnetic spin-models as  $d$  varies between the lower and the upper critical dimensionalities. Our results are consistent with, but more extensive and sometimes more accurate than those obtained from the existing dimer series or from the estimates of related exponents for lattice animals, branched polymers and fluids. We mention also that it is possible to obtain estimates of the dimer constants from our series for the various lattices.

PACS numbers: 05.50.+q, 64.60.De, 75.10.Hk, 03.70.+k

Keywords: Ising model, Yang-Lee edge, Dimer model, Magnetic field

## I. INTRODUCTION

Let us consider a classical spin-1/2 Ising system with nearest-neighbor ferromagnetic interactions, in the presence of an external magnetic field  $H$ , on a finite  $d$ -dimensional lattice of  $N$  sites. The partition function can be written as

$$Z_N(H, T) = \sum_{conf} \exp \left[ K \sum_{\langle ij \rangle} s_i s_j + h \sum_i s_i \right]. \quad (1)$$

Here  $s_i = \pm 1$  denotes an Ising spin variable associated to the site  $i$  of the lattice. The first sum extends to all configurations of the spins, the second to all distinct pairs  $\langle ij \rangle$  of nearest-neighbor spins, the third to all spins. We have set  $K = J/k_B T$ , with  $T$  the temperature,  $J > 0$  the exchange coupling of the spins,  $k_B$  the Boltzmann constant, and  $h = H/k_B T$  the reduced magnetic field. It is a classical result<sup>1,2</sup> that, for real  $T$ ,  $Z_N(H, T)$  has a sequence of zeroes that can occur only on the imaginary axis of the complex  $h = h' + ih''$  plane. This statement remains true for a wide variety of models with ferromagnetic couplings, including Ising models of arbitrary spin<sup>3</sup>,  $n$ -vector models<sup>4-6</sup> (at least for  $n < 4$ ), etc.. As long as the number  $N$  of sites remains finite, these zeroes give rise to a sequence of logarithmic branch-points of the free energy. For  $T$  above its critical value  $T_c$ , when the thermodynamic limit  $N \rightarrow \infty$  is taken, these cuts coalesce into two continuous lines of singularities along the imaginary axis of the  $h$ -plane that extend to infinity and originate at the “Yang-Lee(YL) edges”,  $h'' = \pm h''_{YL}(T)$ , with  $h''_{YL}(T) > 0$ . The partition function must then be nonzero and the free energy must be analytic in a strip containing the real axis of the complex reduced field plane, so that no phase transition can occur for  $T > T_c$ . As  $T \rightarrow T_c$ , we have  $h''_{YL}(T) \rightarrow 0$ , so the gap between the endpoints of the singularity lines shrinks and they tend to pinch the real axis of the complex field plane giving rise, for  $T < T_c$ , to the characteristic discontinuity associated with the spontaneous magnetization.

At fixed  $T > T_c$ , in the vicinity of a YL edge, the magnetization per spin is expected to exhibit a power-law behavior<sup>7</sup>

$$M(H, T) \sim |h \pm ih''_{YL}(T)|^\sigma \quad (2)$$

controlled by an exponent  $\sigma$ .

The main features of these YL edge-singularities have been extensively studied. *A priori* the exponent  $\sigma$  might depend on the temperature and the particular features of the model, however it was observed that it is universal, i.e. it depends only on the spatial dimensionality, but not on the structure of the lattice on which the spin model is defined. Moreover, due to the presence of the magnetic field, this exponent does not depend on the number of components of the spin. Hence for an  $n$ -vector ferromagnetic system, it must be the same as for an Ising system. Finally, the study of solvable models in one dimension or for  $d \rightarrow \infty$  (the mean-field model) or, for any dimension, in the  $n \rightarrow \infty$  limit (the spherical model), and finally the numerical study<sup>7</sup> of non-trivial Ising systems in  $d = 2$  and  $d = 3$  dimensions, indicates that, for  $T > T_c$ , the exponents  $\sigma = \sigma(d)$  are temperature-independent. Due to these universality features, the properties of the YL edges have been related<sup>8</sup> to those of the ordinary critical points in the theory of second-order phase transitions. In this respect, an important step forward was to show that a renormalization-group approach to the calculation of the exponent  $\sigma$  can be formulated<sup>8</sup> in terms of an effective Landau-Ginzburg one-component scalar field theory with a cubic interaction and a purely imaginary

coupling. This entails the upper critical dimensionality  $d_c = 6$ , at and above which the exponent takes its mean-field value  $\sigma = 1/2$ . Moreover  $\sigma$  can be expressed as an expansion in powers of  $\epsilon = 6 - d$ , whose coefficients have been so far computed<sup>8,9</sup> through the third order. See Eq.(12) below.

The interest of an accurate determination of  $\sigma(d)$  is enhanced by the realization that the YL edge exponent is also related to other exponents characterizing the behavior of several quite different systems:

a) The pressure for  $d$ -dimensional fluids, with repulsive-core interactions among their constituents, exhibits an unphysical singularity located at negative values of the activity and showing universal exponents<sup>10-13</sup>  $\phi(d) = \sigma(d) + 1$ . A similar property is true for lattice systems of hard squares (and higher-dimensional solids).

b) The number-per-site of directed branched polymers with  $s$  bonds (or of directed site- or bond-animals<sup>14,15</sup> of size  $s$ ) on a  $d$ -dimensional lattice, has a scaling behavior characterized by a power of  $s$  with universal exponent<sup>16-18</sup>  $\phi_D(d) = \sigma(d - 1) + 1$ . The scaling behavior of the directed branched polymers has been mapped<sup>19</sup> into that of the aforementioned fluids at the unphysical singularity, in one fewer space dimension.

c) The universal exponents characterizing the behavior of the number-per-site of large isotropic branched polymers<sup>20</sup> in a good solvent (or, equivalently<sup>21</sup>, of undirected site- or bond-animals) on a  $d$ -dimensional lattice can be expressed as  $\phi_I(d) = \sigma(d - 2) + 2$ . The scaling behavior of the isotropically branched polymers has been mapped<sup>22</sup> into that, mentioned above, of the fluids in two fewer dimensions.

d) A field theoretic model<sup>23</sup> of the Anderson localization exhibits the same critical behavior as the isotropic branched polymers mentioned above in c).

Refs.[12,24] provide us with tables of numerical estimates of these exponents for the systems of a), b) and c) in spatial dimensionalities  $0 \leq d \leq 8$ , which corroborate these exponent identifications. In particular, estimates of the exponent  $\phi_I(d)$  for high-dimensional undirected site-animals have been obtained from 15th-order activity expansions<sup>24</sup>, and, more recently, have been complemented by extensive MonteCarlo simulations<sup>25</sup> and exact enumerations<sup>26</sup>.

We have recently calculated<sup>27,28</sup>, in most cases through 24th order, the high-temperature(HT) and low-field expansion of the magnetization in an external field for several models in the Ising universality class, including the conventional Ising spin-1/2 model, on a sequence of bipartite lattices of spatial dimensionalities  $2 \leq d \leq 7$ . In this paper, we shall use these data, most not yet existing in the literature, to improve the accuracy and extend the range of direct estimates of the exponents of the YL edge-singularity. Our work is based on the observation<sup>8,29-31</sup> that this task can be accomplished restricting to the study of the Ising magnetization in a particular HT limit, since the exponents  $\sigma(d)$  are temperature-independent. It was shown that, in this limit, for each value of  $d$ , the bivariate expansion of the magnetization in powers of the inverse temperature at low field reduces to a simpler univariate expansion of a quantity related to the density of a dimer system on the same lattice, in powers of a variable  $z$  that can be viewed as the activity of the dimers. Hence, the estimates of the exponents  $\sigma(d)$  can be obtained from the simpler study of a singularity in the complex  $z$ -plane.

The paper is organized as follows. In the second Section, we describe briefly the dimer model and sketch the arguments relating the Ising magnetization and the dimer density. In the third Section, we discuss the numerical estimates of the exponents  $\sigma(d)$ . In the fourth Section, we briefly mention the possibility of obtaining accurate estimates of the dimer

constants from the dimer series for several lattices. In the final Section, we summarize our work and draw some conclusions.

TABLE I: Expansion coefficients  $d_n$  of the dimer density per site  $\rho = \sum_{n=1}^{\infty} d_n z^n$  for various lattices. In the case of the square lattice, the coefficients were already known<sup>31</sup> through order 17, in the simple-cubic lattice case through order 15, in the body-centered-cubic case through order 13.

	sq	sc	bcc
$d_1$	2	3	4
$d_2$	-14	-33	-60
$d_3$	116	438	1096
$d_4$	-1042	-6381	-22076
$d_5$	9812	98298	471384
$d_6$	-95288	-1571646	-10462752
$d_7$	945688	25804572	238712352
$d_8$	-9537906	-432195261	-5559491148
$d_9$	97398764	7351521882	131557495336
$d_{10}$	-1004479624	-126601633818	-3152926387520
$d_{11}$	10442811216	2202345302028	76350685086240
$d_{12}$	-109291830952	-38634960958878	-1864887612147680
$d_{13}$	1150263509280	682589371293612	45882795957148336
$d_{14}$	-12164408791920	-12133302712160964	-1135919635021757184
$d_{15}$	129177146454536	216812614019536368	28273604715543144816
$d_{16}$	-1376741271026898	-3892138971898300893	-707057878652500074156
$d_{17}$	14719835348283940	70154203323444808578	17755217609022707289048
$d_{18}$	-157827022198103624	-1269064065215177023170	-447499139067294036693120
$d_{19}$	1696509872615736256	23030962300401009234828	11315759542146218070302592
$d_{20}$	-18277500804075889672	-419178020538794595807786	-286983128267601041433972576
$d_{21}$	197318358676755340504	7649309116068955304095452	7297713321539491454122083408
$d_{22}$	-2134157389758234716560	-139919791900565246008916796	-186023844148307269386048046560
$d_{23}$	23121845343883130936248	2564949986696274806668222464	4752360937807056276521029006800
$d_{24}$	-250895842743288634987656	-47113178583259985664916986702	-121654579352079670288510647161952

## II. DIMER DENSITY AND ISING MAGNETIZATION

The hard dimer model in two space dimensions was introduced<sup>32</sup> long ago to study the adsorption of diatomic molecules on a regular surface. On a  $d$ -dimensional lattice of  $N$  sites it describes an assembly of linear objects each one covering a single bond of the lattice including the two endpoint sites, under the constraint of no partial or total overlap (*hard* dimers). The statistics of this model is described by the configurational macrocanonical partition function

$$\Xi_N(z) = 1 + \sum_{s=1}^{N/2} g_N(s) z^s. \quad (3)$$

Here  $g_N(s)$  denotes the number of ways of placing  $s$  dimers over the links of the  $N$ -site lattice, and  $z$  is the dimer activity.

In the thermodynamical limit

$$\Xi(z) = \lim_{N \rightarrow \infty} [\Xi_N(z)]^{1/N} = 1 + \sum_{s=1}^{\infty} g(s) z^s \quad (4)$$

TABLE II: Expansion coefficients  $d_n$  of the dimer density per site  $\rho = \sum_{n=1}^{\infty} d_n z^n$ , in the case of the h4sc and of the h4bcc lattices, for which no data exist in the literature.

	h4sc	h4bcc
$d_1$	4	8
$d_2$	-60	-248
$d_3$	1096	9488
$d_4$	-22100	-403528
$d_5$	473064	18295568
$d_6$	-10540512	-865807424
$d_7$	241719216	42249956512
$d_8$	-5664784788	-2109836426376
$d_9$	135024044344	107268694276016
$d_{10}$	-3262426210400	-5532784189984768
$d_{11}$	79709668733952	288753867270427776
$d_{12}$	-1965728629262720	-15218580836786546560
$d_{13}$	48861010499029408	808774465817914713216
$d_{14}$	-1222763683250863968	-43288481720615472507456
$d_{15}$	30780446257662843696	2331290979582407692061408
$d_{16}$	-778830611224069318356	-126230584983092928283366536
$d_{17}$	19796376474243625682760	6867529887763685727515233744
$d_{18}$	-505225273989977429147424	-375209852952369261768265528064
$d_{19}$	12940687836519051181004448	20577462138006148093915106417728
$d_{20}$	-332541786326958137163996960	-1132370504978616213744537711827968
$d_{21}$	8570723905802396225090813040	62506221601565914680638405721677920
$d_{22}$	-221490566192354289867699314976	-3459983056502070079122589397022126400
$d_{23}$	5737972822751243066305678738704	192014799892871528814114123763838125600
$d_{24}$	-148983747147193194624766250874624	-10681019026724387660511023640151016838528

and the macrocanonical potential is defined as

$$\Gamma(z) = \ln(\Xi(z)) = \sum_{s=1}^{\infty} \gamma_s z^s. \quad (5)$$

The dimer density per site  $\rho(z)$  is then expressed in terms of the potential  $\Gamma(z)$  as

$$\rho(z) = z \frac{d\Gamma}{dz} = \sum_{n=1}^{\infty} d_n z^n \quad (6)$$

with  $d_n = n\gamma_n$ . Let us now summarize the simple argument<sup>8,29-31</sup> relating the HT and low-field expansions of the spin-1/2 Ising model in the limit of infinite temperature with the low-density expansions for hard dimers on the same lattice. In the thermodynamical limit, the HT expansion of the Ising magnetization per spin can be written as

$$M(H, T) = c + 2(1 - c^2) \sum_{l=1}^{\infty} \frac{v^l}{l} \sum_{m=1}^l m \psi_{ml} c^{2m-1} \quad (7)$$

with  $v = \tanh(K)$  and  $c = \tanh(h)$ . In the elementary graphical representation of the HT and low-field expansion of the specific free energy, each term of order  $l$  in  $v$  and  $2m$  in  $c$  is associated to a configuration of  $l$  bonds and  $2m \leq 2l$  marked vertices on the lattice. The coefficients surviving in the particular limit in which  $v \rightarrow 0$  and  $c \rightarrow \infty$  with fixed  $z = vc^2$ , are associated to configurations of  $l$  separated bonds whose endpoints are  $2l$  marked vertices

TABLE III: Expansion coefficients  $d_n$  of the dimer density per site  $\rho = \sum_{n=1}^{\infty} d_n z^n$ , in the case of the h5sc and of the h5bcc lattices, for which no data exist in the literature.

	h5sc	h5bcc
$d_1$	5	16
$d_2$	-95	-1008
$d_3$	2210	78880
$d_4$	-56935	-6888560
$d_5$	1560470	643011936
$d_6$	-44589470	-62772421632
$d_7$	1312933060	6328669301376
$d_8$	-39545139015	-653740982885040
$d_9$	1212383059070	68823661085963680
$d_{10}$	-37702721543530	-7356685696560126848
$d_{11}$	1186280544459180	796252824523662796416
$d_{12}$	-37692235412554270	-87086303698430880977408
$d_{13}$	1207600893566962380	9609234910400277365928640
$d_{14}$	-38966834192905441260	-1068376395044310231082721280
$d_{15}$	1265202803884630177880	119569512978084142014703005120
$d_{16}$	-41303509002873877637895	-13459302500635793010903317240880
$d_{17}$	1354882911889343633812990	1522782576346629681778159256296800
$d_{18}$	-44635036629478941618353330	-173070180804086640006367948602645120
$d_{19}$	1476101842809890620493385820	19750115971287989745172871861397745920
$d_{20}$	-48984496236897026046190228810	-2262063795052955748647989801450884168960
$d_{21}$	1630653500450336878870631247220	259942605480019278589477461871133106000960
$d_{22}$	-54438143496599430247473673703380	-29961083663149896944399970822493200812776320
$d_{23}$		3462835569237061144802332732162000087319991360
$d_{24}$		-401237452358873371565154489237992019311699297280

and therefore they are related to the number of ways of placing  $l$  hard dimers on the lattice in such a way that for the magnetization (i.e. the field-derivative of the free energy) one has

$$M(H, T)/c \rightarrow [1 - 2\rho(z)] \quad (8)$$

with

$$\rho(z) = \sum_{l=1}^{\infty} \psi_l z^l \quad (9)$$

the activity expansion of the dimer density.

The behavior eq.(2) of the magnetization nearby the YL edge must translate into

$$\rho(z) \sim |z - z_0|^\sigma \quad (10)$$

for the dimer density, where

$$z_0 = - \lim_{T \rightarrow \infty} (\tan(h''_{YL}(T)))^2 \tanh(K) \quad (11)$$

is a real negative quantity.

### III. THE EXTENDED EXPANSIONS OF THE DIMER DENSITY

Our recent calculation<sup>27,28</sup>, in most cases through order 24, of the HT expansion of the spin-1/2 Ising magnetization in the presence of an external field, for several bipartite lattices

TABLE IV: Expansion coefficients  $d_n$  of the dimer density per site  $\rho = \sum_{n=1}^{\infty} d_n z^n$ , in the case of the h6sc and of the h6bcc lattices, for which no data exist in the literature.

	h6sc	h6bcc
$d_1$	6	32
$d_2$	-138	-4064
$d_3$	3900	643136
$d_4$	-122310	-113792032
$d_5$	4086396	21547360832
$d_6$	-142476792	-4271044245248
$d_7$	5122735176	874932782274688
$d_8$	-188517518310	-183742680108707616
$d_9$	7064821951140	39344571392293056704
$d_{10}$	-268661239644168	-8557358633880518454784
$d_{11}$	10340279507701776	1885218050259702418922496
$d_{12}$	-402003973427568648	-419794129141493673828232192
$d_{13}$	15763048131921626880	94331821844075469462840829440
$d_{14}$	-622646937215063631120	-21363417876150273316847202904320
$d_{15}$	24752424038720810997240	4871104500436454268454972630464896
$d_{16}$	-989526434040322269780870	-1117286822866349754715547920533865248
$d_{17}$	39754803422947748576043180	257621581517072116407677681638058301760
$d_{18}$	-1604239977818820429337772040	-59680091386808879450249399896382705283584
$d_{19}$	64993232282038522127491654560	13883370669662028006386373064762884655595776
$d_{20}$	-2642511808864143082376138558280	-3241891787443021814766940463936149652806538752
$d_{21}$	107788019222920474225378253424840	759601317388101093048127502735990937113754258304
$d_{22}$		-178534783824842834362110547423593615649270807425280
$d_{23}$		42081725576331603416392306775511862130364642844236928
$d_{24}$		-9944795581281129212782166232032493020106438172525218816

of dimensionality  $2 \leq d \leq 7$ , enables us to extend through the same order the expansions of the dimer density in powers of the activity  $z$  on these lattices. Such expansions were already tabulated in the literature<sup>31</sup> in the case of the square(sq)(17 terms), the simple-cubic(sc)(15 terms), the body-centered-cubic(bcc)(13 terms) lattices. The known coefficients are reproduced by our calculation. Actually, a few more coefficients could be derived from the published HT and low-field expansions<sup>35</sup> for the sq(19 terms) and the sc(17 terms) lattices. Also for the hyper-simple-cubic(h4sc) lattice in  $d = 4$  spatial dimensions, 16 correct terms of the free-energy expansion were tabulated<sup>35</sup> in the same paper. However, these data were overlooked in Ref.[31] and in the successive work.

We have extended the activity expansions in the case of the h4sc and the hyper-bcc (h4bcc) lattices in  $d = 4$  spatial dimensions through the 24th order. Our calculation for the higher-dimensional hyper-bcc lattices extends also through the 24th order, whereas in the case of the five- and six-dimensional hsc lattices, it reaches only the 22nd and the 21st, respectively. For dimension  $d = 7$ , our expansion on the hsc lattice extend only to the 20th order. These data were not yet available in the literature.

The expansions for the h5sc, h6sc,...,h7sc lattices have been truncated at a slightly smaller order, because on the (hyper-)cubic lattices the computation of the embedding numbers for the highest-order graphs is too time-consuming to be completed in just a few days by a single personal computer. While in the case of the hbcc lattices the computational complexity of the calculation is independent<sup>27</sup> of the lattice dimensionality, in the hsc case it grows exponentially with the space dimensionality.

We have not yet extended the calculation of the series in the cases of non-bipartite lattices

TABLE V: Expansion coefficients  $d_n$  of the dimer density per site  $\rho = \sum_{n=1}^{\infty} d_n z^n$ , in the case of the seven-dimensional sc and bcc lattices, for which no data exist in the literature.

	h7sc	h7bcc
$d_1$	7	64
$d_2$	-189	-16320
$d_3$	6286	5193856
$d_4$	-232337	-1849727936
$d_5$	9156882	705432330624
$d_6$	-376866798	-281737586952192
$d_7$	16002790188	116325399366292992
$d_8$	-695763137601	-49250328402750744768
$d_9$	30814814722594	21265341161536087474816
$d_{10}$	-1385226427142474	-9328024156759223705208320
$d_{11}$	63037109428097196	4145112005630262044731153920
$d_{12}$	-2898142120281195662	-1862040622714788094682263408640
$d_{13}$	134406753861096711820	844180535052646908871372654226176
$d_{14}$	-6280176867758451284340	-385755924146309028765643631630290940
$d_{15}$	295357093420022257715616	177488316175328670895488110020974226176
$d_{16}$	-13970161606657482586444833	-82155985773613044917541164342517378676416
$d_{17}$	664121988815559152932012890	38231156319654300832459678139949723942242688
$d_{18}$	-31713748014463596772472407794	-17875202142357193337368185100702670312872235520
$d_{19}$	1520542773828098297725351871436	8393167978080707171882156986310088446859172518912
$d_{20}$	-73169317004302689750290322402042	-3956035371299664049518526770009878297187847196261376
$d_{21}$		1871101505460166042039514382404078383796375971968146688
$d_{22}$		-887773576351504314786611216702175344355035369163473610240
$d_{23}$		422432182192613348318985610505592297395940532680091395006720
$d_{24}$		-201538729427533378265902478728701415730702344267711209153902592

such as the triangular, face-centered-cubic and their high-dimensional generalizations. The coefficients of our extended expansions of the dimer density series for  $2 \leq d \leq 7$  are reported in the Tables I... V.

#### IV. ANALYSIS OF THE DIMER EXPANSIONS

For the dimer density series, we have located the nearest negative singularity in the complex  $z$ -plane and estimated its exponent  $\sigma$  by the numerical tools currently used to extrapolate the behavior of power expansions to the border of their analyticity disk, in particular employing the *differential approximants* (DAs). These are a generalization of the well known Padé approximant (PA) method that approximates the series under study by the solution of an ordinary inhomogeneous linear differential equation with polynomial coefficients. For a detailed illustration of their definitions, of their properties, and for a general discussion of the uncertainties in the estimates of the singularity parameters determined by this method, we address the reader to Refs.[15,27,28,36].

Let us first consider the few known terms of the  $\epsilon$ -expansion of the exponent  $\sigma$

$$\sigma(d) = \frac{1}{2} - \frac{1}{12}\epsilon - \frac{79}{3888}\epsilon^2 + \left(\frac{1}{81}\zeta(3) - \frac{10445}{1250712}\right)\epsilon^3 + O(\epsilon^4) \quad (12)$$

where  $\zeta(n)$  denotes the Riemann zeta function. The expansion eq.(12) can be resummed following various procedures, all yielding consistent results for  $1 < d < 6$ . For example, several simple continuous interpolations of  $\sigma(d)$  with respect to the space dimensionality



$d$ , can be found<sup>12,31</sup> in the literature, which are obtained from low-order constrained Padé approximants. The continuous curve in Fig.1, is the plot vs  $d$  of a  $[3/2]$  Padé approximant formed from the  $\epsilon$ -expansion eq.(12), that satisfies the additional constraints of reproducing the known exact values<sup>37</sup>  $\sigma(2) = -1/6$  for  $d = 2$  and  $\sigma(1) = -1/2$  at the lower critical dimension  $d = 1$ . For  $d > 6$ , the exponent should retain the value  $\sigma(d) = 1/2$  and so this part of the curve is drawn flat. The constrained  $[3/2]$  PA has the expression

$$\sigma(d) = \frac{-0.00564924115\epsilon^3 - 0.141867697\epsilon^2 + 0.390189052\epsilon + 1/2}{-0.0852567479\epsilon^2 + 0.947044730\epsilon + 1}. \quad (13)$$

The resummation by this approximant is visually indistinguishable from that obtained by the  $[6/0]$  PA subject to the constraint of reproducing the exact results for  $d = 0, 1, 2$ . The latter approximation was proposed in Ref.[12] to describe the behavior of the exponents of the unphysical singularity at negative activity for repulsive-core fluids as  $d$  varies. Alternative, but completely consistent interpolations can be obtained by other more refined resummation procedures<sup>9</sup>, including a Padé-Borel method and a conformal mapping technique. For each dimension  $d$ , the small spread among the estimates of  $\sigma(d)$  obtained by the various resummations methods of the expansion eq.(12) can be used to roughly limit an interval of possible values of  $\sigma(d)$ , whose width increases with  $\epsilon$ . We have reported these spreads in the eighth column of Table VI.

An  $\epsilon$ -expansion through the third order has been computed<sup>12</sup> also for the leading correction-to-scaling exponent  $\theta(d)$ . Its values  $\theta(2) = 0.83(1)$ ,  $\theta(3) = 0.622(12)$ ,  $\theta(4) = 0.412(8)$  and  $\theta(5) = 0.205(5)$  for the various dimensions have been estimated<sup>12</sup> by constrained PAs. Here we shall use these estimates without further discussion.

From these studies of the  $\epsilon$ -expansion, we are thus led to expect that the exponent  $\sigma(d)$  should lie between  $\sigma = -1/2$ , its  $d = 1$  value, and  $\sigma = 1/2$ , the  $d = 6$  value. For intermediate values of  $d$ , the exponent should take values not far from those suggested by the various resummation procedures. In conclusion,  $\sigma(d)$  is expected to take small and possibly positive values for  $2 < d < 6$ . The DAs are probably unable to measure accurately exponents in this range of values and therefore, as suggested in Ref.[31], it is more convenient to analyze the  $z$ -derivative of the dimer density, rather than  $\rho(z)$  itself, because it has a sharper singularity, characterized by the exponent  $\sigma - 1$ .

Our procedure of numerical analysis is the following. To begin with, we determine a central value  $z_0$  of the location of the singularity by averaging over an appropriate sample of estimates from first- or second-order DAs, selected among those using most or all available series coefficients. Evident outliers are excluded from the sample. The uncertainty attached to  $z_0$  is a small multiple of the spread of the reduced sample. Then we can evaluate also the corresponding exponent  $\sigma(d)$  using a sample of second- or third-order DAs which are *biased* with the previously determined central value  $z_0$ , i.e. are built to be singular at  $z_0$ . This computational procedure allows only partially for the influence of the expected corrections to scaling on the estimates of the exponent, just because the DAs are more flexible than PAs. However the estimates so obtained still suggest a significant residual influence of the corrections to scaling, which is especially relevant in the case of the (hyper)-sc lattices and for large dimensionalities, and so we have tried to further improve our accuracy using also the well known procedure<sup>12,38</sup> of evaluating the exponent after performing the variable transformation

$$w = 1 - (1 - z/z_0)^{\theta(d)} \quad (14)$$

on the series. By this simple prescription, the leading non-analytic correction to scaling of the

TABLE VI: Estimates of the location  $z_0$  and the exponent  $\sigma(d)$  of the nearest singularity of the dimer density in the complex activity plane  $z$  for several bipartite lattices of dimension  $2 \leq d \leq 7$ . In the first column, we have indicated the structure and dimensionality of the lattice. The second and fourth column show the results of Ref.[31], while the third and fifth contain the results of this paper. Notice that, for  $d \geq 5$ , our estimates for the hsc lattices are based on shorter series. In the sixth column, we have reported the values of  $\sigma(d) = \phi(d) - 1$  obtained<sup>12</sup> from the exponent occurring for repulsive-core fluids. In the seventh column, we have shown estimates<sup>25</sup> of the exponent  $\sigma(d) = \phi_I(d+2) - 2$  derived from a high-precision MonteCarlo simulation of site-animals. In the eighth column, we have indicated ranges of estimates of  $\sigma$  obtained from different resummation prescriptions of the  $\epsilon$ -expansion. The last column reports exact results for  $\sigma$ , whenever known. The data in the last two columns depend only on the lattice dimensionality.

lattice	$z_0$ (Ref.[31])	$z_0$ (Our work)	$\sigma$ (Ref.[31])	$\sigma$ (Our work)	Fluids (Ref.[12])	Animals (Ref.[25])	$\sigma$ $\epsilon$ -exp.(Ref.[9])	$\sigma$ Exact
sq	-0.088962(1)	-0.0889642(2)	-0.1645(20)	-0.1662(5)	-0.161(8)	-0.165(6)	0.146-0.166	-1/6
tri	-0.056076(2)		-0.1620(15)					
sc	-0.052002(6)	-0.0520268(2)	0.096(6)	0.077(2)	0.0877(25)	0.080(7)	0.079-0.091	
bcc	-0.037309(4)	-0.0373125(2)	0.090(5)	0.076(2)				
fcc	-0.02413(18)		0.097(11)					
h4sc		-0.0365624(4)		0.258(5)	0.2648(15)	0.261(12)	0.262-0.266	
h4bcc		-0.0170399(2)		0.261(4)				
h5sc		-0.0281849(4)		0.401(9)	0.402(5)	0.40(2)	0.399-0.400	
h5bcc		-0.00814235(4)		0.402(2)				
h6sc		-0.0229462(6)		0.460(50)	0.465(35)		1/2	1/2
h6bcc		-0.0039832(2)		0.475(30)				
h7sc		-0.019360(3)		0.495(8)				1/2
h7bcc		-0.0019715(3)		0.498(3)				

given series is approximately changed into an analytic one, which should be more accurately dealt with by the DAs. We observe that generally the estimates show little sensitivity to small variations of the bias value of  $z_0$  and of the correction exponents  $\theta(d)$ , so that our final uncertainties can generously allow also for the spreads of these input parameters.

The estimates of the singularity location  $z_0$  in the activity plane and of the exponent  $\sigma(d)$  obtained by this kind of analysis are shown in the third and fifth columns of Table VI and compared with those from a previous accurate DA analysis<sup>31</sup> of activity expansions shorter than those now available, that was performed along similar lines, but not explicitly allowing for the corrections to scaling. Our results generally lie within the range roughly suggested by the resummed  $\epsilon$ -expansion and are essentially consistent with the existing pure DA estimates<sup>29,31</sup> for  $d < 4$ , but are more precise. It is worth to stress that our expansions of the dimer-density cover the whole range of dimensionalities between the lower and the upper critical dimension and therefore our results are also more extensive. For comparison, in the Table VI for each value of  $d$ , we have also reported estimates of  $\sigma(d)$  obtained<sup>12</sup> from the exponents  $\phi(d)$  associated to repulsive-core fluids and estimates obtained from the exponents  $\phi_I(d+2)$  associated to the undirected site animals in  $d+2$  dimensions. The former data were obtained<sup>12</sup> by a DA analysis (which allowed for the corrections to scaling) of the 14th-order fugacity-expansions for a model of a binary molecular mixture, with Gaussian interaction, in dimensions  $1 \leq d \leq 6$ . The latter data were more recently obtained<sup>25</sup> by extensive MonteCarlo simulations performed in the case of (hyper)-simple-cubic lattices with  $2 \leq d \leq 9$ . Both sets of estimates are essentially consistent with our results within their (sometimes larger) uncertainties.

It is also worth noticing that, if we allow explicitly for the corrections to scaling using the variable transformation defined by eq.(14), our estimates of  $\sigma(3)$  are somewhat smaller than the older results<sup>31</sup> from shorter dimer series, show a closer agreement with the constrained PA resummation of the  $\epsilon$ -expansion and exhibit more accurately the expected universality with respect to the lattice structure. The universality check is satisfactory also in  $d = 4$ . For  $d = 5$  dimensions, the check is still as accurate, in spite of the small leading correction exponent, because of which other unaccounted higher corrections to scaling might also be significant.

At the upper critical dimension  $d_c = 6$ , it is expected that the power singularity of the dimer density is multiplicatively corrected<sup>12,39,40</sup> by a power of a logarithm and that moreover also the leading corrections to scaling are logarithmic. Since the DAs are notoriously unfit to describe accurately this kind of singularity, it is not surprising that their convergence deteriorates. For lack of established and effective prescriptions to deal with this computation, we cannot do better than assigning to the estimate of  $\sigma(6)$ , an uncertainty much larger than the apparent spread of DAs.

For completeness, we have computed  $\sigma(d)$  also for the higher-dimensional hsc and hbcc lattices just to check that, as expected, above the upper critical dimension, the exponents  $\sigma(d)$  retain the mean-field value, so that  $\sigma(7) = 1/2$ , etc.. For graphical convenience, we have reported in the figure only the seven-dimensional result.

In the Fig.1, we have always reported the weighted average of the estimates for the sc- and the bcc-type lattices and attached to it a small multiple of the largest uncertainty of the single results.

## V. DIMER CONSTANTS

Let us now show briefly that sufficiently long low-activity expansions of the dimer density can be of use also in estimating heuristically the constant  $h_d$  that controls the exponential growth of the number of all possible dimer arrangements over the bonds of a  $N$ -site  $d$ -dimensional simple-cubic lattice in the large  $N$  limit. This quantity is defined by

$$h_d = \ln \left[ \lim_{N \rightarrow \infty} (\Xi_N(z))^{1/N} \right]_{z=1} = \Gamma(1) \quad (15)$$

and is often called *monomer-dimer constant* of the lattice under study, the term *monomer* referring to a site unoccupied by a dimer.

It is more difficult to get from the series data good estimates also for the constant that characterizes the exponential growth of the number of the closely-packed dimer coverings (i.e. dimer arrangements such that every lattice site belongs to a dimer) for a  $N$ -site  $d$ -dimensional simple-cubic lattice in the large  $N$  limit,

$$\tilde{h}_d = \lim_{z \rightarrow \infty} [\Gamma(z) - \rho(z) \ln z]. \quad (16)$$

The quantity  $e^{\tilde{h}_d}$  is often called *molecular freedom*.

The constants<sup>41</sup>  $h_d$  and  $\tilde{h}_d$  (which of course have nothing to do with the reduced magnetic field mentioned in the Introduction), are of interest in chemistry, combinatorial mathematics and information theory, but unfortunately their exact values are not known except<sup>42-44</sup> in the case of  $\tilde{h}_2$ . In particular, the quantities  $h_2$ ,  $h_3$ ,  $h_4$  and  $h_5$  are known rigorously only through their bounds.

Consider first the computation of  $h_d$ . In the case of the sq lattice, a naive [12,12] PA of the  $z$ -expansion of  $\Gamma(z)$  yields the estimate  $h_2 \approx 0.662798\dots$ . This result agrees to six significant digits with the most precise determination<sup>45,46</sup>  $h_2 = 0.6627989727(1)$  and is consistent with the tightest presently known bounds  $0.66279897190 \leq h_2 \leq 0.662798972844913$ . Other accurate, but also non-rigorous estimates of  $h_2$  can be found in the literature<sup>29,47–51</sup>. In particular Ref.[50] reports a twelve figure determination of this constant.

By the same quite simple prescription, in the case of the sc lattice, we find  $h_3 \approx 0.7859\dots$ , a value which lies between the known<sup>52</sup> bounds:  $0.7849602275 \leq h_3 \leq 0.7862023450$ . For the h4sc lattice, our PA estimate is  $h_4 \approx 0.880\dots$ , which should be compared with the lower bound<sup>46</sup>  $0.8638570485$ . These results show that very naive PAs yield rather accurate analytic continuations of the  $z$ -expansion of  $\Gamma(z)$  well outside its very small convergence disk. The precision of the estimates decreases as the space dimension  $d$  grows simply because the radius of convergence  $|z_0|$  of the  $z$ -expansion of  $\Gamma(z)$  vanishes as  $d$  grows (see Table VI).

Unfortunately, this straightforward approach does not provide an analytic continuation of  $\Gamma(z)$  of acceptable accuracy for  $z \gg 1$ , that is necessary to compute also  $\tilde{h}_d$ . We can try to mitigate this difficulty, performing in the  $z$ -expansion the simple change<sup>33,49</sup> of variable  $z = t/(1 - (q - 1)t)^2$ , where  $q$  is the coordination number of the lattice under study. As a first result, we can observe a drastic improvement in the apparent accuracy of the aforementioned estimates of the constants  $h_d$ . For example, we obtain  $h_2 \approx 0.662798972\dots$ , which reproduces three additional digits of the best estimate of  $h_2$ . For the three-dimensional sc lattice, the improved estimate is  $h_3 \approx 0.7859660\dots$  and in four dimensions we obtain  $h_4 \approx 0.88071788\dots$ . For the five-dimensional cubic lattice:  $h_5 \approx 0.958123\dots$ , consistently with the known lower bound  $0.94383303 \leq h_5$ . Let us also stress that for the five- (and higher-dimensional) hsc lattices our expansions are slightly shorter. For example, they extend only through the 22nd order in the five-dimensional hsc case.

Correspondingly, we have computed the values of the dimer density per site for  $z = 1$  obtaining:  $\rho_2(1) \approx 0.31906155\dots$  (in complete agreement with the estimates of Ref.[45,47]),  $\rho_3(1) \approx 0.3421901\dots$ ,  $\rho_4(1) \approx 0.3579234\dots$  and  $\rho_5(1) \approx 0.369580\dots$ . Other estimates for higher-dimensional hsc lattices and for the hbcc lattices can also be found in Table VII. For  $d > 3$ , our estimates of  $h_d$  for the hsc lattices compare well with the lower bounds provided by the inequality<sup>46,52</sup>

$$h_d \geq \frac{1}{2}[-p \ln p - 2(1 - p) \ln(1 - p) + p \ln 2d - p] \quad (17)$$

with  $p = \frac{4d+1-\sqrt{8d+1}}{4d}$ . The meaning of the estimates of  $h_d$ , summarized in Table VII, is the following: we have reported only the decimal figures which appear to be stabilized in the three highest-order diagonal PAs that can be formed from the available dimer expansions.

In terms of the new variable, the potential  $\Gamma(z)$  can be, with a better approximation, continued by PAs into a larger region of the complex  $z$ -plane, encompassing intermediate values of  $z$  such as  $z \approx 10$ . We have tried to infer the large  $z$  limit of the quantity  $\Gamma(z) - \rho(z) \ln z$  in eq.(16) by observing that, in the intermediate  $z$  region, this quantity behaves linearly in  $1/\sqrt{z}$  to a fair approximation, and extrapolating this behavior to  $z = \infty$ . We can thus conjecture estimates of the constants  $\tilde{h}_d$ , that although generally reasonable and consistent with the known<sup>46</sup> bounds, unsurprisingly show an accuracy much lower than in the  $h_d$  case and therefore will not be reported in the Table VII. The blame for this failure lays on the still insufficient extension of the region of accurate analytic continuation and the arbitrariness of the various extrapolation procedures, that make a safe evaluation of the uncertainties difficult.

TABLE VII: Our estimates of the dimer constants  $h_d$  and the corresponding estimates of the dimer densities  $\rho_d(1)$  (third column) for (hyper-)simple-cubic and (hyper-)body-centered-cubic lattices of various dimensionalities. In the second column we have reported lower bounds and in the fourth upper bounds for  $h_d$  on the hsc lattice when available. No bounds are known for the hbcc lattices. In the text we have reported also estimates by other authors, when existing.

hsc	Lower limit	This work	Upper limit	hbcc	This work
$h_2$	0.66279897190	0.662798972(1)	0.662798972844913		
$\rho_2(1)$		0.31906155(1)			
$h_3$	0.7849602275	0.7859660(1)	0.7862023450	$h_3$	0.8813479(1)
$\rho_3(1)$		0.3421901(1)		$\rho_3(1)$	0.3584362(1)
$h_4$	0.8638570485	0.880718(1)		$h_4$	1.131880(1)
$\rho_4(1)$		0.3579234(1)		$\rho_4(1)$	0.392552(1)
$h_5$	0.94383303	0.95813(1)		$h_5$	1.408080(1)
$\rho_5(1)$		0.369580(1)		$\rho_5(1)$	0.420248(1)
$h_6$	1.01129436	1.023732(1)		$h_6$	1.703890(2)
$\rho_6(1)$		0.37868106(1)		$\rho_6(1)$	0.4417731(1)
$h_7$	1.06972606	1.080759(2)		$h_7$	2.0142(2)
$\rho_7(1)$		0.38604998(2)		$\rho_7(1)$	0.457881(2)

## VI. CONCLUSIONS

We have derived the coefficients of the series expansions of the dimer density in powers of the activity, in most cases through 24th-order, for several bipartite lattices of dimensionality  $2 \leq d \leq 7$ . Thus we have not only extended the existing series data, so far published only for  $d \leq 3$ , but also produced series for  $d \geq 4$ . An analysis of this set of data improves the accuracy in the determination of the locations and the exponents of the nearest real negative singularity of the dimer density in the complex activity plane. The exponents controlling the Yang-Lee edge-singularity of this class of ferromagnetic spin models in a wide range of space dimensions are related, in some cases by a simple dimensionality shift, with the exponents characterizing very different systems. The numerical estimates presently available for all these exponents show a good consistency among them and with the results of appropriate resummations of the renormalization-group  $\epsilon$ -expansion. Our dimer-density series are also shown to be of some use in estimating the dimer constants  $h_d$  and  $\tilde{h}_d$ .

## VII. ACKNOWLEDGEMENTS

We are grateful to A.J. Guttmann for reading a preliminary draft. We are also grateful to P.H.Lundow and K. Markström for helpful comments on the final Section of the paper. We thank the Physics Departments of Milano-Bicocca University and of Milano University for hospitality and support. Partial support by the MIUR is also acknowledged.

---

\* Electronic address: paolo.butera@mib.infn.it

† Electronic address: mario.pernici@mi.infn.it

<sup>1</sup> C.N. Yang and T.D. Lee, Phys. Rev. **87**, 404 (1952).

<sup>2</sup> T.D. Lee and C.N. Yang, Phys. Rev. **87**, 410 (1952).

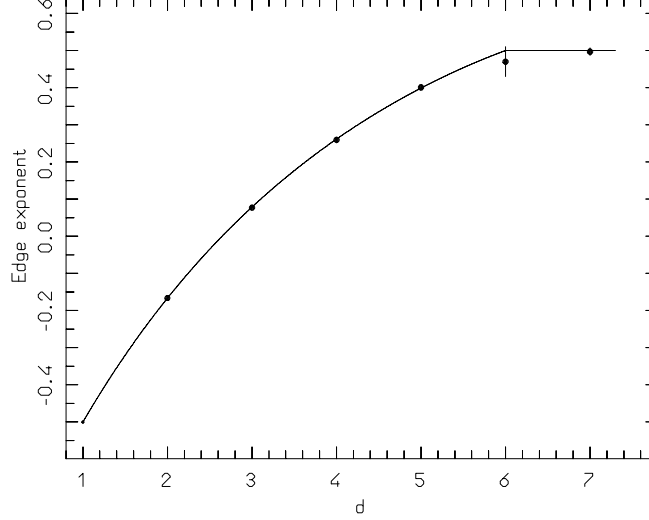


FIG. 1: Estimates (full circles) of the edge-exponent  $\sigma(d)$ , obtained our dimer density expansions vs the lattice dimensionality. The continuous curve is obtained resumming the third order  $\epsilon$ -expansion of  $\sigma(d)$  by a  $[3/2]$  Padé approximant constrained to reproduce the exactly known values of the exponent for  $d = 1$  and  $d = 2$ .

- <sup>3</sup> R.B. Griffiths, J. Math. Phys. **10**, 1559 (1969).
- <sup>4</sup> F. Dunlop and C. M. Newman, Commun. Math. Phys., **44**, 223 (1975).
- <sup>5</sup> C. M. Newman, J. Stat. Phys. **15**, 399 (1976).
- <sup>6</sup> E. H. Lieb and A. D. Sokal, Commun. Math. Phys. **80**, 153 (1981).
- <sup>7</sup> P.J. Kortman and R.B. Griffiths, Phys. Rev. Lett. **27**, 1439 (1971).
- <sup>8</sup> M.E. Fisher, Phys. Rev. Lett. **40**, 1610 (1978).
- <sup>9</sup> O.F. de Alcantara Bonfin, J.E. Kirkham and A.J. McKane, J.Phys. A **14**, 2391 (1981).
- <sup>10</sup> D. Poland, J. Stat. Phys. **35**, 341 (1984).
- <sup>11</sup> A. Baram and M. Luban, Phys. Rev. A **36**, 760 (1987).
- <sup>12</sup> S.N. Lai and M.E. Fisher, J. Chem. Phys. **103**, 8144 (1995).
- <sup>13</sup> Y. Park and M.E. Fisher, Phys. Rev. E **60**, 6323 (1999).
- <sup>14</sup> D. Stauffer and A. Aharony, “*Introduction to Percolation Theory*”, 2nd edition, (Taylor and Francis, London 1994).
- <sup>15</sup> A.J. Guttmann, in “*Polygons, Polyominoes and Polycubes*”, edited by A.J. Guttmann. Lecture Notes in Physics, vol. 775, (Springer New York, 2009).
- <sup>16</sup> J.L. Cardy, J. Phys. A **15**, L593 (1982).
- <sup>17</sup> H.E. Stanley, S.Redner and Z.R. Yang, J.Phys. A **15**, L569 (1982).
- <sup>18</sup> N. Breuer and H. K. Janssen, Z. Phys. B **48**, 347 (1982).
- <sup>19</sup> J.Z. Imbrie, J. Phys. A **37**, L137 (2004).
- <sup>20</sup> G. Parisi and N. Surlas, Phys. Rev. Lett. **46**, 871 (1981).
- <sup>21</sup> T.C.Lubensky and J. Isaacson, Phys. Rev. Lett. **41**, 829 (1978).
- <sup>22</sup> D.C. Brydges and J.Z. Imbrie, J. Stat. Phys. **110**, 503 (2003).
- <sup>23</sup> T.C.Lubensky and A. Mc Kane, J. Physique (France) Lett. **42**, L331 (1981).
- <sup>24</sup> J. Adler, Y. Meir, A. B. Harris, A. Aharony and J.A.M.S. Duarte, Phys. Rev. B **38**, 4941 (1988).
- <sup>25</sup> H.P. Hsu, W. Nadier and P. Grassberger, J. Phys. A **38**, 775 (2005).

- <sup>26</sup> S. Luther and S. Mertens, J. Stat. Mech. P09026 (2011).
- <sup>27</sup> P. Butera and M. Pernici, Phys. Rev. B **83**, 054433 (2011).
- <sup>28</sup> P. Butera and M. Pernici, Phys. Rev. E **85**, 021105 (2012).
- <sup>29</sup> D.S. Gaunt, Phys. Rev. **179**, 174 (1969).
- <sup>30</sup> G.A. Baker Jr. and P. Moussa, J. Appl. Phys. **49**, 1360 (1978).
- <sup>31</sup> D.A. Kurtze and M.E. Fisher, Phys. Rev. B **20**, 2785 (1979).
- <sup>32</sup> R. H. Fowler and G. S. Rushbrooke, Trans. Faraday Soc. **33**, 1272 (1937).
- <sup>33</sup> O.J. Heilmann and E.H. Lieb, Commun. Math. Phys. **25**, 190 (1972).
- <sup>34</sup> C. Gruber and H. Kunz, Commun. Math. Phys. **22**, 133 (1971).
- <sup>35</sup> S. McKenzie, Can. J. Phys., **57**, 1239 (1979).
- <sup>36</sup> A.J. Guttmann, in “*Phase Transitions and Critical Phenomena*” edited by C. Domb and J. L. Lebowitz, vol. 13, page 1, (Academic Press, New York 1989).
- <sup>37</sup> J.L. Cardy, Phys. Rev. Lett. **54**, 1354 (1985).
- <sup>38</sup> R.Z. Roskies, Phys. Rev. B **23**, 6037 (1981).
- <sup>39</sup> J.J. Ruiz-Lorenzo, J. Phys. A **31**, 8773 (1998).
- <sup>40</sup> C. Ferber, D. Foster, H. P. Hsu and R. Kenna, Eur. Phys. J. B **83**, 245 (2011).
- <sup>41</sup> S. R. Finch, *Mathematical constants*, Cambridge University Press (2003).
- <sup>42</sup> P.W. Kasteleyn, Physica **27**, 1209 (1961).
- <sup>43</sup> H. N. V. Temperley and M.E. Fisher, Phil. Mag. **6**, 1061 (1961).
- <sup>44</sup> M.E. Fisher, Phys. Rev. **124**, 1664 (1961).
- <sup>45</sup> R.J. Baxter, J. Math. Phys. **9**, 650 (1968).
- <sup>46</sup> S. Friedland and U.N. Peled, Adv. Appl. Math. **34**, 486 (2005).
- <sup>47</sup> L. K. Runnels, J. Math. Phys. **11**, 842 (1970).
- <sup>48</sup> I. Beichl, D.P. O’Leary, and F. Sullivan, Phys. Rev. E **64**, 016701 (2001).
- <sup>49</sup> J. F. Nagle, Phys. Rev. **152**, 190 (1966).
- <sup>50</sup> Y. Kong, Phys. Rev. E **74**, 061102 (2006).
- <sup>51</sup> Yan Huo, Heng Liang, Si-Qi Liu, and Fengshan Bai, Phys. Rev. E **77**, 016706 (2008).
- <sup>52</sup> S. Friedland, E. Krop, P.H. Lundow and K. Markström, J. Stat. Phys. **133**, 513 (2008).